

# Optimizing the performance of thermionic devices using energy filtering

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Conventional thermionic power generators and refrigerators utilize a barrier in the direction of transport to selectively transmit high-energy electrons. Here we show that the energy spectrum of electrons transmitted in this way is not optimal, and we derive the ideal energy spectrum for operation in the maximum power regime. By using suitable energy filters, such as resonances in quantum dots, the power of thermionic devices can, in principle, be improved by an order of magnitude.

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Thermionic power generators [1, 2, 3] utilize a temperature difference between two reservoirs of electrons to transport high-energy electrons against an electrochemical potential gradient. By increasing the applied voltage between the reservoirs, the same device can operate in reverse as a refrigerator [4, 5, 6, 7, 8, 9], using the electrochemical potential difference to remove high-energy ('hot') electrons from the colder reservoir. The required energy selectivity is conventionally achieved by a barrier between the hot and cold reservoirs (Fig. 1). Thermionic devices may be distinguished from thermoelectric devices by the use of a barrier which is narrower than the electron mean free path (ballistic transport) [3]. For the purposes of this paper, it is important to note that the 'energy barriers' used in conventional devices may more precisely be called ' $k_x$  barriers', as they actually constrain the *momentum* of electrons transmitted in direction of transport so that  $k_x \geq k'_x$ . While all electrons with energies less than  $E_B = (\hbar k'_x)^2 / 2m$  are blocked by such a barrier, *not all electrons with  $E \geq E_B$  are transmitted*. In contrast, an 'energy filter' may be understood to be a mechanism which selectively transmits electrons in a particular range of  $E = (\hbar k)^2 / 2m$ , where  $k^2 = k_x^2 + k_y^2 + k_z^2$ . To illustrate this difference, we show in figure 1(b) a Fermi sphere, representing in momentum space the occupation of states of a free electron gas. The shaded volume (segment) shows the range of electrons transmitted in the positive  $x$  direction by a ' $k_x$  barrier'. For comparison, the electrons transmitted by an 'energy filter' correspond to a 'shell' in  $k$  space, as illustrated in Fig 2 (b).

In this paper we show that, from a fundamental point of view, the use of a ' $k_x$  barrier' is not the best possible design for a thermionic device. We begin by briefly reviewing how energy filtering can be used to achieve maximum *efficiency* in thermionic devices [10]. Based upon these results, we find the energy spectrum of electrons

FIG. 1: (a) Schematic of a conventional thermionic device, consisting of two electron reservoirs with different temperatures and electrochemical potentials. An intervening energy barrier of height  $E_B = (\hbar k'_x)^2 / 2m$  constrains the momentum of electrons in the direction of transport to those with  $k_x \geq k'_x$ . For relatively low voltages, there are more high-energy electrons on the hot side of the barrier, and power is generated by a net electron flow from the hot to the cold reservoirs. If the voltage is increased, the number of high-energy electrons on the cold side of the barrier increases. At some voltage the net current direction reverses, and the device cools the cold reservoir by removing "hot" electrons. (b) Fermi sphere where the segment for which  $k_x \geq k'_x$  has been shaded.

that must be transmitted to achieve maximum power, and so obtain expressions for the theoretical maximum power of thermionic power generators and refrigerators, respectively. Finally we compare this ideal case to the spectrum of electrons actually transmitted by conventional devices using a  $k_x$  barrier, finding an order of magnitude increase in the maximum power obtainable from an idealized energy-filtered device compared to a similarly idealized device which uses a  $k_x$  barrier.

Hot carrier solar cells [11, 12], quantum dot cryogenic refrigerators [13, 14] and quantum Brownian heat engines [10, 15] that employ energy filters have been proposed. It has been shown that ballistic transport of electrons between two reservoirs of free electron gas is an isentropic

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FIG. 2: (a) At the energy  $E_0$ , defined by Eq. 1, the Fermi distributions in the two reservoirs are equal,  $f_C(E_0) = f_H(E_0)$ . The letter G indicates the energy range ( $E_0 < E < \infty$ ) for which electrons flow spontaneously from hot to cold, and where power generation occurs. In the range R ( $\varepsilon_C < E < E_0$ ) electrons flow from cold to hot and remove heat from the cold reservoir. (b) Fermi sphere showing the thin shell of electrons transmitted by an energy filter.

process at the energy

$$E_0 = \frac{\varepsilon_C T_H - \varepsilon_H T_C}{T_H - T_C} \quad (1)$$

where the Fermi distributions,  $f_{H/C}(E_0) = [1 + \exp([E_0 - \varepsilon_{H/C}]/kT_{H/C})]^{-1}$ , in the hot (H) and cold (C) reservoirs are equal [10, 15]. For power generation, this energy fulfills the condition  $W = \eta Q_{in}$  [11, 12], where  $W = (\varepsilon_C - \varepsilon_H)$  is the work done by each electron transported from the hot to the cold reservoirs against the electrochemical potential difference,  $Q_{in} = (E_0 - \varepsilon_H)$  is the heat removed from the hot reservoir by an electron with energy  $E_0$ , and  $\eta = (1 - T_C/T_H)$  is the ‘Carnot factor’, the maximum fraction of heat which may be transformed into useful work by a heat engine working between temperatures  $T_H$  and  $T_C$ . For refrigeration,  $E_0$  fulfills the condition  $Q_{out} = W [T_C/(T_H - T_C)]$ , where  $[T_C/(T_H - T_C)]$  is the coefficient of performance of a reversible refrigerator and  $Q_{out} = (E_0 - \varepsilon_C)$  is the heat removed by an electron with energy  $E_0$  from the cold reservoir.

At  $E_0$ , transport of electrons is reversible and there is no thermodynamically spontaneous direction for current to flow. A device which only allowed electrons with this energy to be transmitted would operate with Carnot efficiency but zero power [10, 15]. To find the energy spectrum of electrons which should be transmitted for maximum power, we note that power is generated whenever electrons flow from the hot to the cold reservoir. On the other hand, the cold reservoir is refrigerated when electrons from above the electrochemical potential in the cold reservoir flow to the hot reservoir. Over what energy ranges do electrons flow from the hot to the cold reservoirs and vice-versa?

To proceed, we assume the availability of an idealized energy filter which transmits all electrons in a desired energy range which arrive at the interface between reservoirs, and we neglect phonon heat leaks. Using spherical

polar coordinates and working in  $k$ -space, the particle current density,  $dj_H$ , of electrons with momentum in the infinitesimal range  $dk$  around  $k$  arriving at the reservoir interface from the hot reservoir is given by

$$dj_H(k) = 2 \int_0^\pi \int_{-\pi/2}^{\pi/2} g(\theta, \phi, k) v_x(\theta, \phi, k) f_H(k) d\theta d\phi dk \quad (2)$$

where the density of states is  $g = (2\pi)^{-3} k^2 \sin\theta d\theta d\phi dk$ , the velocity of electrons in the  $x$  direction (perpendicular to the reservoir interface) is  $v_x = \hbar m^{-1} k \sin\phi \cos\theta$  and the factor of 2 accounts for electron spin. A similar expression can be written for the particle current density  $dj_C$  of electrons arriving at the interface from the cold reservoir. The net particle current density of electrons from the hot to the cold reservoirs is then given by  $dj = (dj_H - dj_C)$ . Evaluating the integral over  $\phi$  and  $\theta$ , and changing variables to  $E = (\hbar k)^2/2m$ , we obtain

$$dj(E) = \frac{mE}{2\pi^2 \hbar^3} [f_H(E) - f_C(E)] dE \quad (3)$$

Assuming that  $T_H > T_C$  and  $\varepsilon_C > \varepsilon_H$ , then  $[f_H(E) - f_C(E)]$  is positive for  $E > E_0$ , and  $dj > 0$ . This means that electrons in the range  $E_0 < E < \infty$  flow from the hot to the cold reservoirs and do work  $W = (\varepsilon_C - \varepsilon_H)$  each, while electrons transmitted below  $E_0$  actually reduce the power, each consuming work  $W$  as they flow in the ‘wrong’ direction from the cold to the hot reservoirs. The theoretical maximum power which can be obtained from a ballistic electron power generator is therefore

$$P_G = (\varepsilon_C - \varepsilon_H) \int_{E_0}^{\infty} dj(E). \quad (4)$$

Below  $E_0$ ,  $f_H(E) < f_C(E)$ , and  $dj(E) < 0$ , so electrons flow from the cold to the hot reservoirs. In order to refrigerate the cold reservoir transmitted electrons must satisfy  $E > \varepsilon_C$  as well, as the heat change  $dQ_C$  in the cold reservoir upon removing an electron with energy  $E$  is given by  $dQ_C = E - \varepsilon_C$ . Electrons with  $E > E_0$  flow from hot to cold, heating the cold reservoir. The theoretical maximum power which can be obtained from a ballistic electron refrigerator is therefore

$$P_R = - \int_{\varepsilon_C}^{E_0} (E - \varepsilon_C) dj(E). \quad (5)$$

We now compare these theoretical limits to the maximum power which may be obtained from an idealised, conventional thermionic device which utilizes a  $k_x$  barrier. We assume complete transmission for all available electrons with  $k_x > k'_x$  (see Fig. 1) and zero transmission

for electrons with  $k_x < k'_x$ , and find

$$P_G^{Con} = (\varepsilon_C - \varepsilon_H) \int_{E_B}^{\infty} (1 - E_B/E) dj(E) \quad (6)$$

$$P_R^{Con} = - \int_{E_B}^{\infty} (1 - E_B/E) (E - \varepsilon_C) dj(E) \quad (7)$$

where  $E_B = (\hbar k'_x)^2/2m$ . The multiplicative term  $(1 - E_B/E)$  is a geometrical factor which occurs due to the fact that only *partial* shells of constant  $k$  are transmitted by devices utilizing a  $k_x$  barrier.

This factor makes the integrand in Equations 6 and 7 smaller than that in Equations 4 and 5 respectively, for all electron energies, so  $P_G^{Con} < P_G$  and  $P_R^{Con} < P_R$ . For the refrigeration regime there is an additional source of non-ideality in the use of a  $k_x$  barrier which is an important consideration when  $eV \lesssim kT$ . In this case there is substantial occupation of states above  $E_0$ , and transmission of electrons with  $E > E_0$  by a  $k_x$  barrier results in a ‘backcurrent’ of hot electrons flowing from the hot to the cold reservoirs, reducing the refrigerating power below the theoretical maximum, given by Equation 5. As an illustrative example, for parameter values of  $T_H = 400$  K,  $T_C = 300$  K,  $eV = 12$  meV ( $\approx 0.5kT_C$ ) and  $m = 0.5m_e$  (where  $m_e$  is the mass of a free electron), and taking  $E_B = E_0$  for power generation,  $P_G/P_G^{Con} = 17$ . Taking  $E_B = \varepsilon_C$  for the refrigeration case, and  $T_H = 300$  K,  $T_C = 265$  K, and the same voltage and effective mass as before,  $P_R/P_R^{Con} = 60$ .

The *efficiency* of an energy filtered power generator working at maximum power (Eq. 4) is also higher than that of a device utilizing a  $k_x$  barrier, as a larger proportion of transmitted electrons have energies close to  $E_0$  [15]. This increase in efficiency is due to the fact that

while all electrons transmitted from the hot to the cold reservoirs do work  $\varepsilon_C - \varepsilon_H$ , electrons close to  $E_0$  do this work more efficiently than higher energy electrons (which remove more heat from the hot reservoir than the minimum required by the second law of thermodynamics). In the refrigeration regime, the efficiency of an energy filtered device working at maximum power is also higher than that of a conventional device when  $eV \lesssim kT$ , due to the suppression of the back-current of high energy electrons. For the device parameters considered above, the efficiency of the energy filtered power generator is 42% of the Carnot limit, while that of the conventional device is 34% of the Carnot limit. The efficiency of the energy filtered electron refrigerator is 23% of the Carnot limit, compared to 22% of the Carnot limit for a conventional device. Note that the efficiency of an energy filtered device can be increased by reducing the range of energies transmitted to  $E_0 - \delta E < E < E_0$ , for refrigeration, or  $E_0 < E < E_0 + \delta E$ , for power generation. When  $\delta E \rightarrow 0$ , the Carnot limit is obtained [10, 15].

In principle, suitable energy filtering for electrons could be implemented via resonant tunnelling through quantum dots [13, 16]. A significant practical loss mechanism for solid-state thermionic devices is thermal conduction via phonons. In an energy filtered device, this problem could potentially be tackled via the multilayer approach suggested by Mahan et al. [3], to develop a device conceptually similar to that of Summers and Brennan [17], or by producing a hybrid vacuum/solid-state device which incorporated nano-scale voids [18] together with quantum dots at reservoir interfaces. A hybrid vacuum/solid-state approach is particularly promising given that the thermal conductivity of nano-porous silicon ( $\sim 0.05$  W m<sup>-1</sup> K<sup>-1</sup> [19]) is comparable to that of materials such as Bi<sub>2</sub>Te<sub>3</sub> ( $\sim 0.07$  W m<sup>-1</sup> K<sup>-1</sup> [20]), commonly used in thermoelectric devices.

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